

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal611txm

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 Feb 24 PCTGEN now available on STN  
NEWS 4 Feb 24 TEMA now available on STN  
NEWS 5 Feb 26 NTIS now allows simultaneous left and right truncation  
NEWS 6 Feb 26 PCTFULL now contains images  
NEWS 7 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results  
NEWS 8 Mar 24 PATDPAFULL now available on STN  
NEWS 9 Mar 24 Additional information for trade-named substances without  
structures available in REGISTRY  
NEWS 10 Apr 11 Display formats in DGENE enhanced  
NEWS 11 Apr 14 MEDLINE Reload  
NEWS 12 Apr 17 Polymer searching in REGISTRY enhanced  
NEWS 13 Jun 13 Indexing from 1947 to 1956 added to records in CA/CAPLUS  
NEWS 14 Apr 21 New current-awareness alert (SDI) frequency in  
WPIDS/WPINDEX/WPIX  
NEWS 15 Apr 28 RDISCLOSURE now available on STN  
NEWS 16 May 05 Pharmacokinetic information and systematic chemical names  
added to PHAR  
NEWS 17 May 15 MEDLINE file segment of TOXCENTER reloaded  
NEWS 18 May 15 Supporter information for ENCOMPPAT and ENCOMPLIT updated  
NEWS 19 May 19 Simultaneous left and right truncation added to WSCA  
NEWS 20 May 19 RAPRA enhanced with new search field, simultaneous left and  
right truncation  
NEWS 21 Jun 06 Simultaneous left and right truncation added to CBNB  
NEWS 22 Jun 06 PASCAL enhanced with additional data  
NEWS 23 Jun 20 2003 edition of the FSTA Thesaurus is now available  
NEWS 24 Jun 25 HSDB has been reloaded  
NEWS 25 Jul 16 Data from 1960-1976 added to RDISCLOSURE  
NEWS 26 Jul 21 Identification of STN records implemented  
NEWS 27 Jul 21 Polymer class term count added to REGISTRY  
NEWS 28 Jul 22 INPADOC: Basic index (/BI) enhanced; Simultaneous Left and  
Right Truncation available  
  
NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT  
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that

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specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 11:22:56 ON 30 JUL 2003

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:23:30 ON 30 JUL 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 JUL 2003 HIGHEST RN 557055-78-4

DICTIONARY FILE UPDATES: 29 JUL 2003 HIGHEST RN 557055-78-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

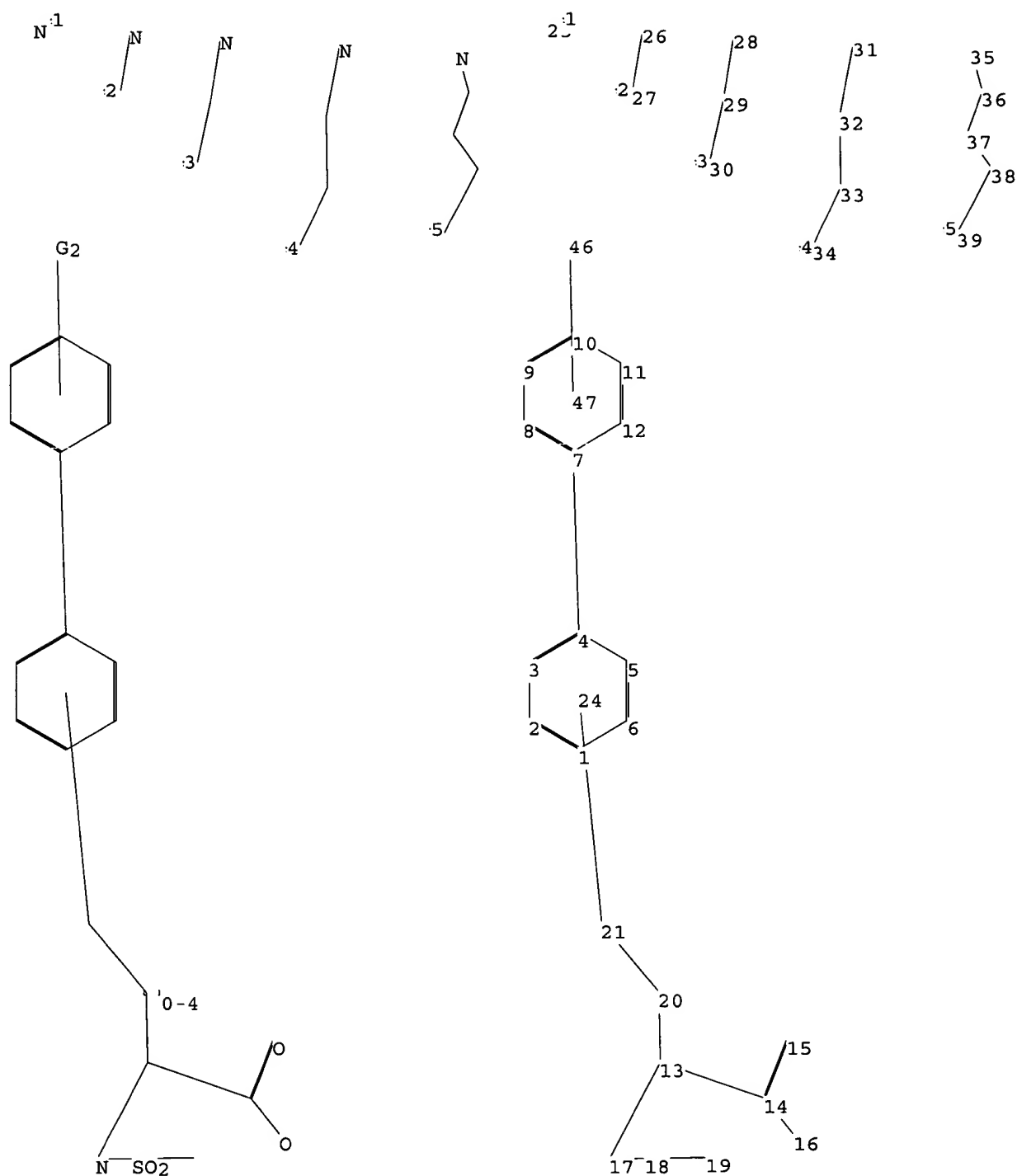
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

Uploading C:\Program Files\Stnexp\Queries\09868305.str



chain nodes :  
 13 14 15 16 17 18 20 21 25 26 27 28 29 30 31 32 33 34 35 36 37  
 38 39 46  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11 12  
 ring/chain nodes :  
 19

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chain bonds :

4-7 13-14 13-20 13-17 14-15 14-16 17-18 18-19 20-21 26-27 28-29 29-30  
31-32 32-33 33-34 35-36 36-37 37-38 38-39

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

13-17 14-15 14-16 17-18 26-27 28-29 31-32 35-36

exact bonds :

4-7 13-14 13-20 18-19 20-21 29-30 32-33 33-34 36-37 37-38 38-39

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G2:[\*1],[\*2],[\*3],[\*4],[\*5]

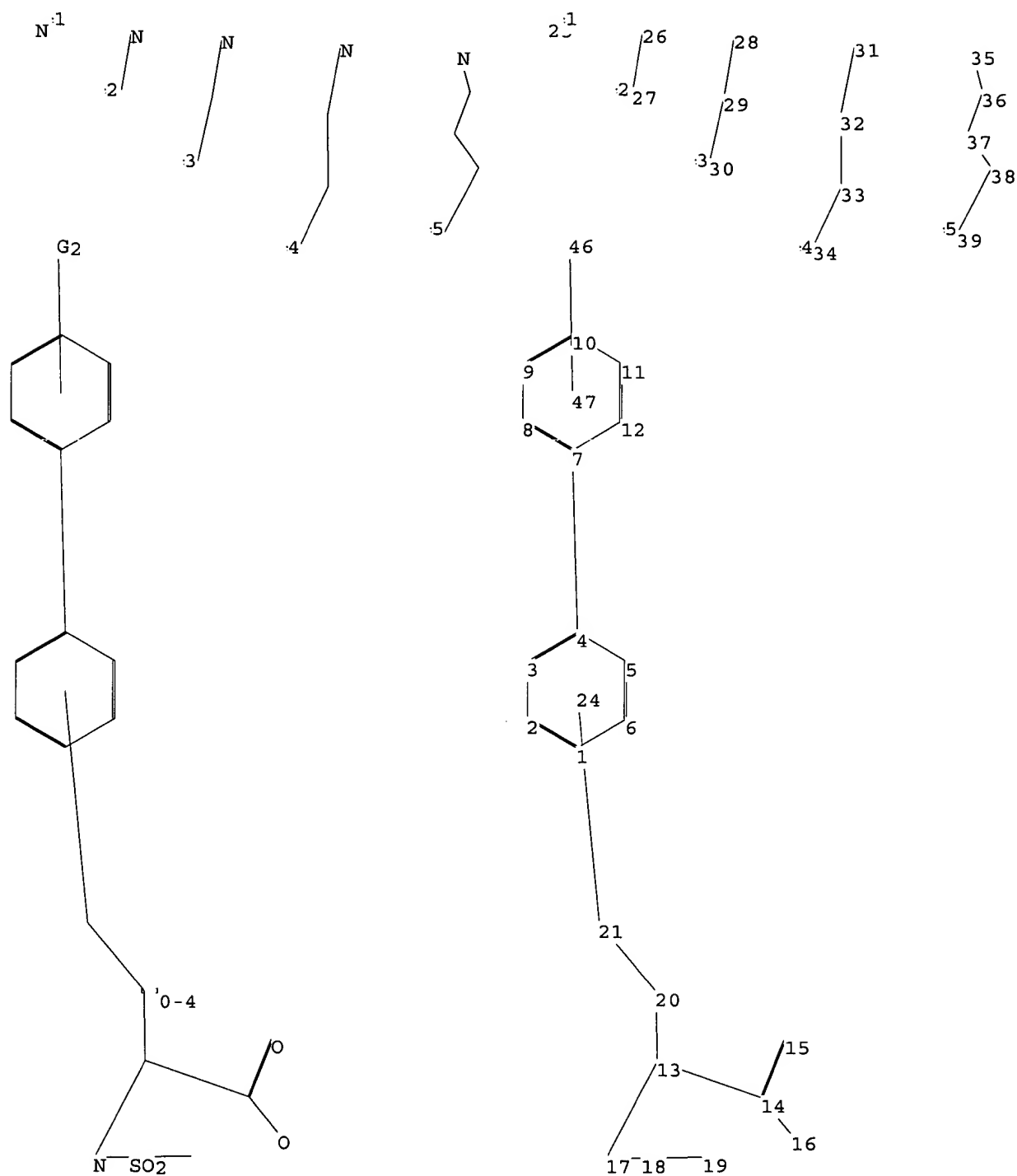
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:CLASS 21:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS  
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS  
37:CLASS 38:CLASS 39:CLASS 46:CLASS 47:CLASS

L1 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\09868305.str



chain nodes :

13 14 15 16 17 18 20 21 25 26 27 28 29 30 31 32 33 34 35 36 37  
38 39 46

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

19

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chain bonds :

4-7 13-14 13-20 13-17 14-15 14-16 17-18 18-19 20-21 26-27 28-29 29-30  
31-32 32-33 33-34 35-36 36-37 37-38 38-39

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

13-17 14-15 14-16 17-18 26-27 28-29 31-32 35-36

exact bonds :

4-7 13-14 13-20 18-19 20-21 29-30 32-33 33-34 36-37 37-38 38-39

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G2:[\*1],[\*2],[\*3],[\*4],[\*5]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:CLASS 21:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS  
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS  
37:CLASS 38:CLASS 39:CLASS 46:CLASS 47:CLASS

L2 STRUCTURE UPLOADED

=> s l2

SAMPLE SEARCH INITIATED 11:24:21 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 74 TO ITERATE

100.0% PROCESSED 74 ITERATIONS  
SEARCH TIME: 00.00.01

15 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

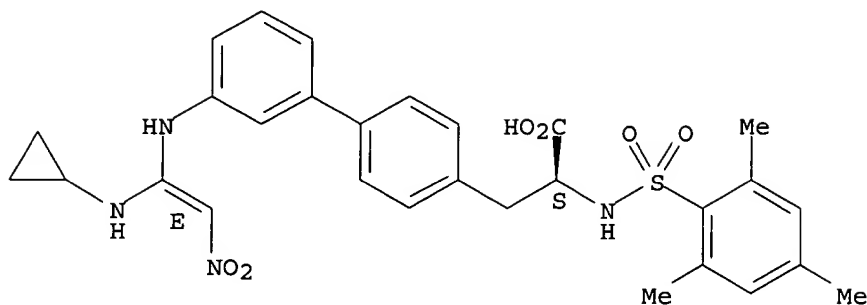
PROJECTED ITERATIONS: 964 TO 1996  
PROJECTED ANSWERS: 68 TO 532

L3 15 SEA SSS SAM L2

=> d scan

L3 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
IN [1,1'-Biphenyl]-4-propanoic acid, 3'-[[ (1E)-1-(cyclopropylamino)-2-nitroethenyl]amino]- $\alpha$ -[[ (2,4,6-trimethylphenyl)sulfonyl]amino]-, ( $\alpha$ S)- (9CI)  
MF C29 H32 N4 O6 S

Absolute stereochemistry.  
Double bond geometry as shown.

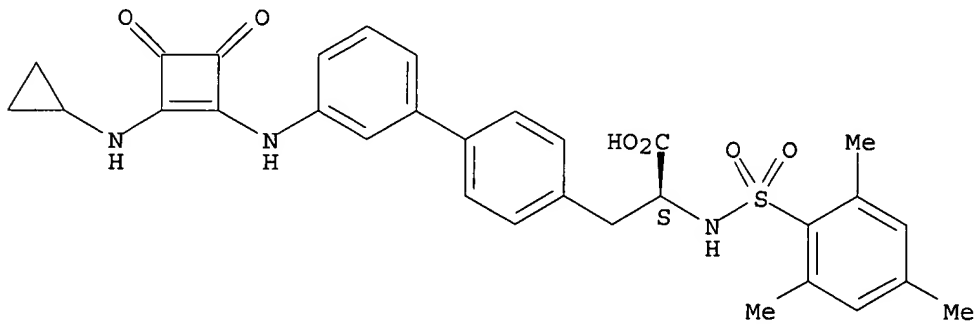


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

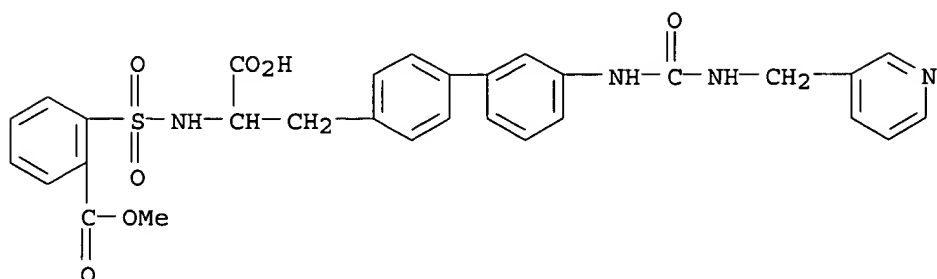
L3 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
 IN [1,1'-Biphenyl]-4-propanoic acid, 3'-[[2-(cyclopropylamino)-3,4-dioxo-1-cyclobuten-1-yl]amino]- $\alpha$ -[[2,4,6-trimethylphenyl)sulfonyl]amino]-, (S) - (9CI)  
 MF C31 H31 N3 O6 S

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
 IN [1,1'-Biphenyl]-4-propanoic acid,  $\alpha$ -[[[2-(methoxycarbonyl)phenyl)sulfonyl]amino]-3'-[[[(3-pyridinylmethyl)amino]carbonyl]amino]- (9CI)  
 MF C30 H28 N4 O7 S

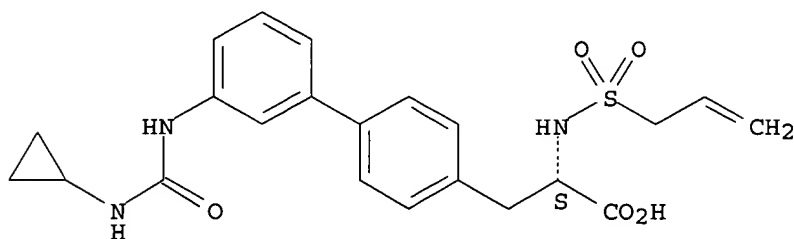


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
 IN [1,1'-Biphenyl]-4-propanoic acid, 3'-[[[(cyclopropylamino)carbonyl]amino]-  
 $\alpha$ -(2-propenylsulfonyl)amino]-, ( $\alpha$ S)- (9CI)  
 MF C22 H25 N3 O5 S

Absolute stereochemistry.



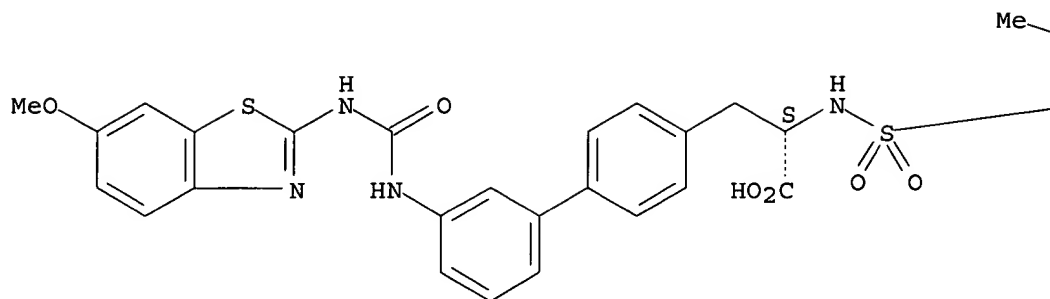
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
 IN [1,1'-Biphenyl]-4-propanoic acid, 3'-[[[(6-methoxy-2-benzothiazolyl)amino]carbonyl]amino]- $\alpha$ -[[[(2,4,6-trimethylphenyl)sulfonyl]amino]-, ( $\alpha$ S)- (9CI)  
 MF C33 H32 N4 O6 S2

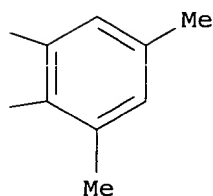
Absolute stereochemistry.



PAGE 1-A



PAGE 1-B



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s 12

SAMPLE SEARCH INITIATED 11:28:26 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 74 TO ITERATE

100.0% PROCESSED 74 ITERATIONS  
SEARCH TIME: 00.00.01

15 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 964 TO 1996  
PROJECTED ANSWERS: 68 TO 532

L4 15 SEA SSS SAM L2

=> s 12 full

FULL SEARCH INITIATED 11:28:33 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1291 TO ITERATE

100.0% PROCESSED 1291 ITERATIONS  
SEARCH TIME: 00.00.01

255 ANSWERS

L5 255 SEA SSS FUL L2

=> file caplus  
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
151.35	151.56

FULL ESTIMATED COST

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FILE 'CAPLUS' ENTERED AT 11:28:42 ON 30 JUL 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 30 Jul 2003 VOL 139 ISS 5  
FILE LAST UPDATED: 29 Jul 2003 (20030729/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l5

L6 3 L5

=> l6 not wo-200035864?/pn

L6 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s l6 not wo-200035864?/pn

1 WO-200035864?/PN  
(WO2000035864/PN)

L7 2 L6 NOT WO-200035864?/PN

=> d 1-2 cbib pi hitstr

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

2002:107924 Document No. 136:167692 Preparation of new biphenyl and biphenyl-analogous compounds as integrin antagonists. Albers, Markus; Urbahns, Klaus; Vaupel, Andrea; Harter, Michael; Schmidt, Delf; Stelte-Ludwig, Beatrix; Gerdes, Christoph; Stahl, Elke; Keldenich, Jorg; Brueggemeier, Ulf; Lustig, Klemens (Germany). U.S. Pat. Appl. Publ. US 2002016461 A1 20020207, 256 pp., Division of U.S. Ser. No. 464,237. (English). CODEN: USXXCO. APPLICATION: US 2001-828514 20010406. PRIORITY: US 1998-PV172225 19981216; US 1999-464237 19991215.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
------------	------	------	-----------------	------

PI	US 2002016461	A1	20020207	US 2001-828514	20010406
	US 6420396	B1	20020716	US 1999-464237	19991215

IT 276257-75-1P 276257-76-2P 276257-77-3P  
276257-78-4P 276257-79-5P 276257-80-8P  
276257-81-9P 276257-82-0P 276257-83-1P  
276257-84-2P 276257-85-3P 276257-86-4P  
276257-87-5P 276257-88-6P 276257-89-7P  
276257-90-0P 276257-91-1P 276257-92-2P  
276257-93-3P 276257-94-4P 276257-95-5P  
276257-96-6P 276257-97-7P 276257-98-8P

L7 ANSWER 18 OF 32 CAPLUS COPYRIGHT 2003 ACS

1996:445595 Document No. 125:137462 N,N'-bisformyl dityrosine is an in vivo precursor of the yeast ascospore wall. Briza, Peter; Kalchhauser, Hermann; Pittenauer, Ernst; Allmaier, Guenter; Breitenbach, Michael (Institut Genetik und Allgemeine Biologie, Universitaet Salzburg, Salzburg, A-5020, Austria). European Journal of Biochemistry, 239(1), 124-131 (English) 1996. CODEN: EJBCAI. ISSN: 0014-2956. Publisher: Springer.

IT 179555-54-5P 179798-22-2P 179798-23-3P

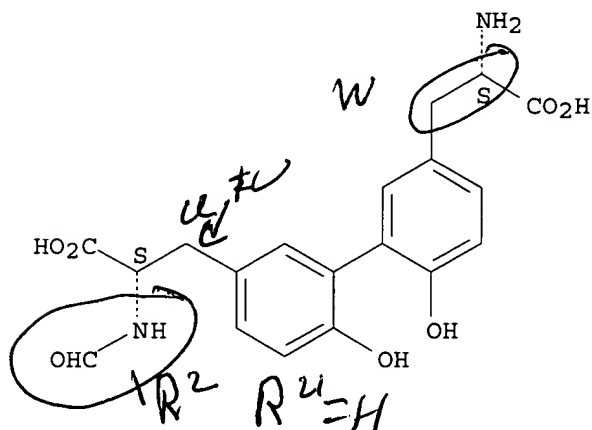
RL: BOC (Biological occurrence); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)

(N,N'-bisformyl dityrosine is in vivo precursor of yeast ascospore wall)

RN 179555-54-5 CAPLUS

CN [1,1'-Biphenyl]-3,3'-dipropanoic acid,  $\alpha$ -amino- $\alpha'$ -(formylamino)-6,6'-dihydroxy-, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

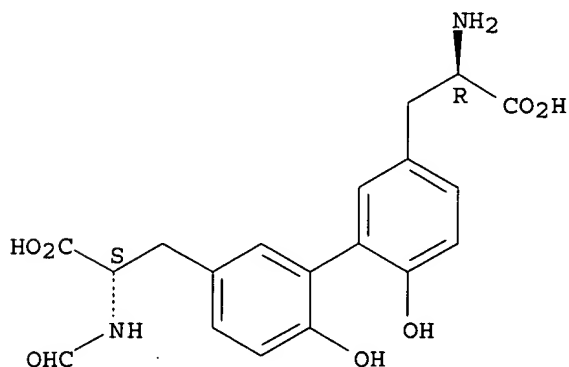
Absolute stereochemistry.



RN 179798-22-2 CAPLUS

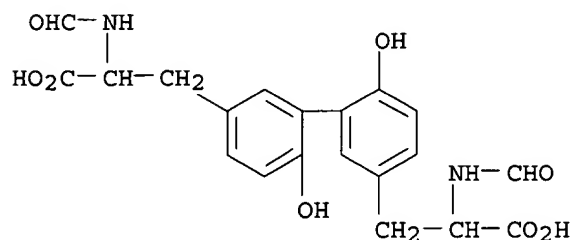
CN [1,1'-Biphenyl]-3,3'-dipropanoic acid,  $\alpha$ -amino- $\alpha'$ -(formylamino)-6,6'-dihydroxy-, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 179798-23-3 CAPLUS

CN [1,1'-Biphenyl]-3,3'-dipropanoic acid,  $\alpha,\alpha'$ -bis(formylamino)-  
6,6'-dihydroxy- (9CI) (CA INDEX NAME)



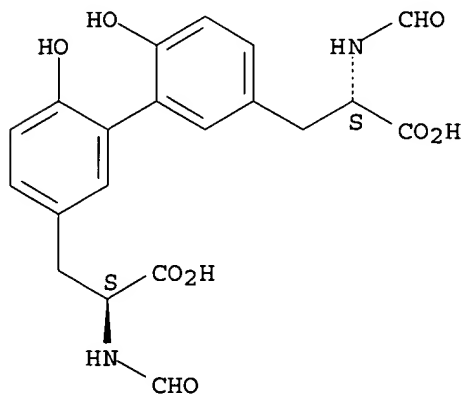
IT 114137-09-6

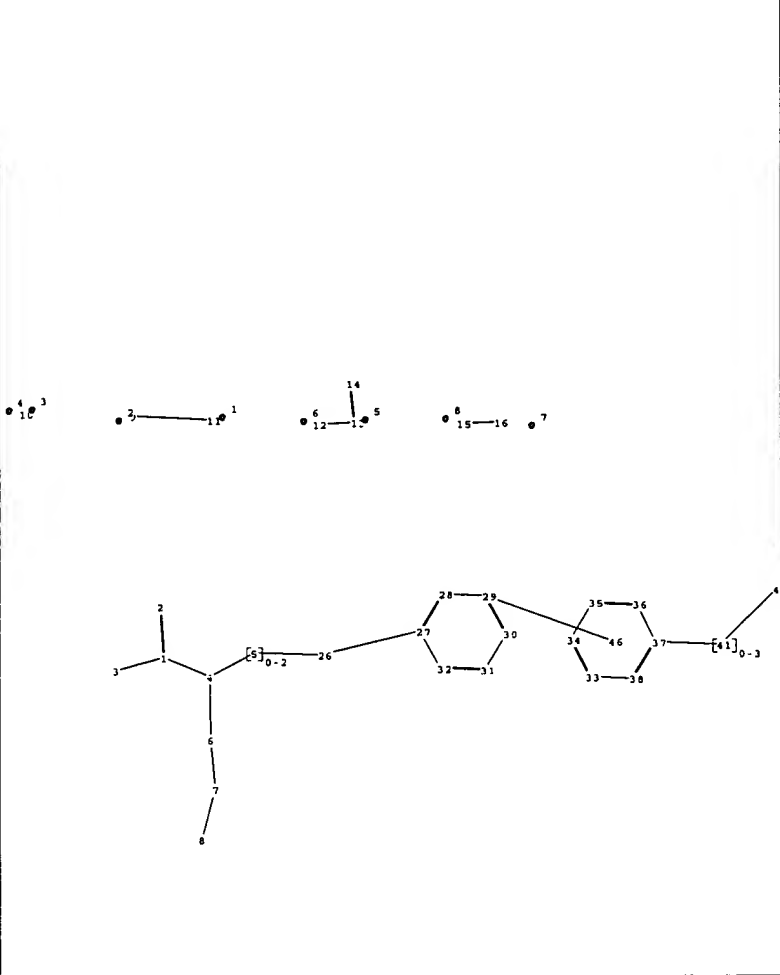
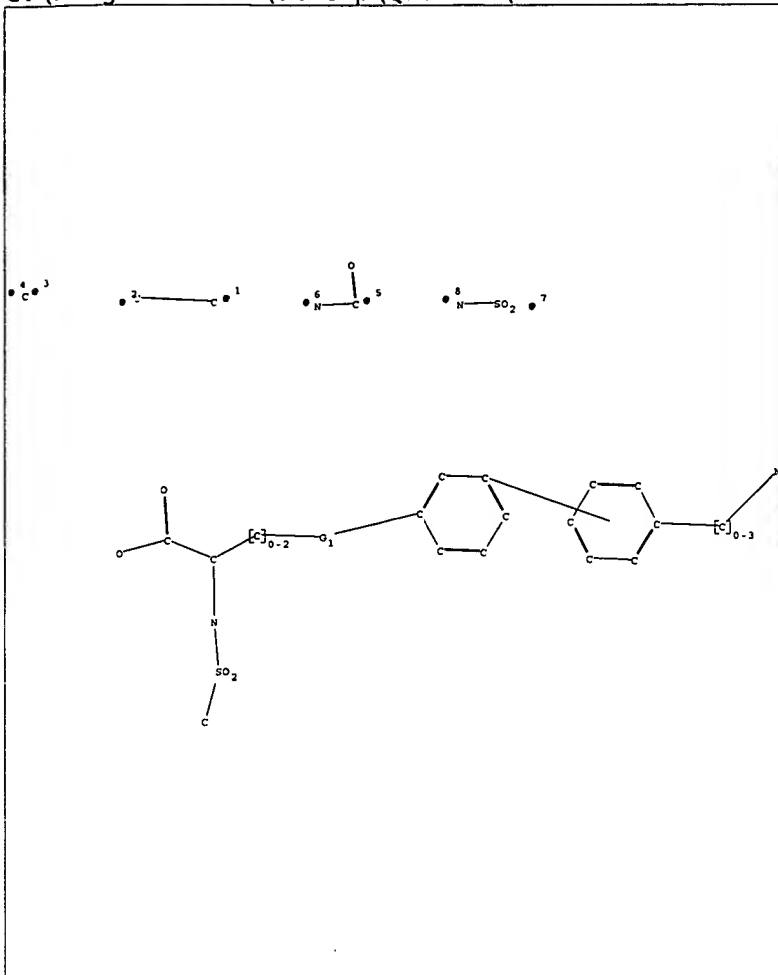
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)  
(N,N'-bisformyl dityrosine is in vivo precursor of yeast ascospore wall)

RN 114137-09-6 CAPLUS

CN [1,1'-Biphenyl]-3,3'-dipropanoic acid,  $\alpha,\alpha'$ -bis(formylamino)-  
6,6'-dihydroxy-, ( $\alpha S,\alpha' S$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





chain nodes :

1 2 3 4 5 6 7 9 10 11 12 13 14 15 16 26 41

ring nodes :

27 28 29 30 31 32 33 34 35 36 37 38

ring/chain nodes :

8 42

chain bonds :

1-2 1-3 1-4 4-5 4-6 5-26 6-7 7-8 9-11 12-13 13-14 15-16 26-27 37-41 41-42

ring bonds :

27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38

exact/norm bonds :

1-2 1-3 4-6 5-26 6-7 12-13 13-14 15-16 26-27 41-42

exact bonds :

1-4 4-5 7-8 9-11 37-41

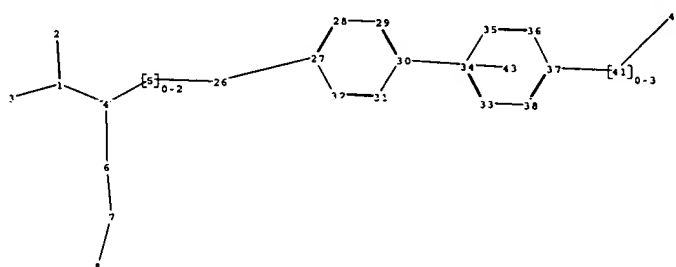
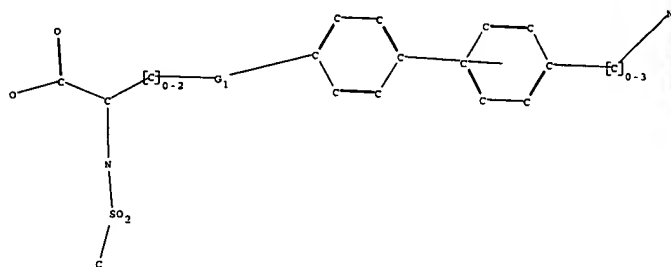
normalized bonds :

27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38

G1:[\*1-\*2],[\*3-\*4],[\*5-\*6],[\*7-\*8]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 26:CLASS 27:Atom 28:Atom  
29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom  
41:CLASS 42:CLASS 46:CLASS



chain nodes :

1 2 3 4 5 6 7 9 10 11 12 13 14 15 16 26 41

ring nodes :

27 28 29 30 31 32 33 34 35 36 37 38

ring/chain nodes :

8 42

chain bonds :

1-2 1-3 1-4 4-5 4-6 5-26 6-7 7-8 9-11 12-13 13-14 15-16 26-27 37-41 41-42

ring bonds :

27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38

exact/norm bonds :

1-2 1-3 4-6 5-26 6-7 12-13 13-14 15-16 26-27 41-42

exact bonds :

1-4 4-5 7-8 9-11 37-41

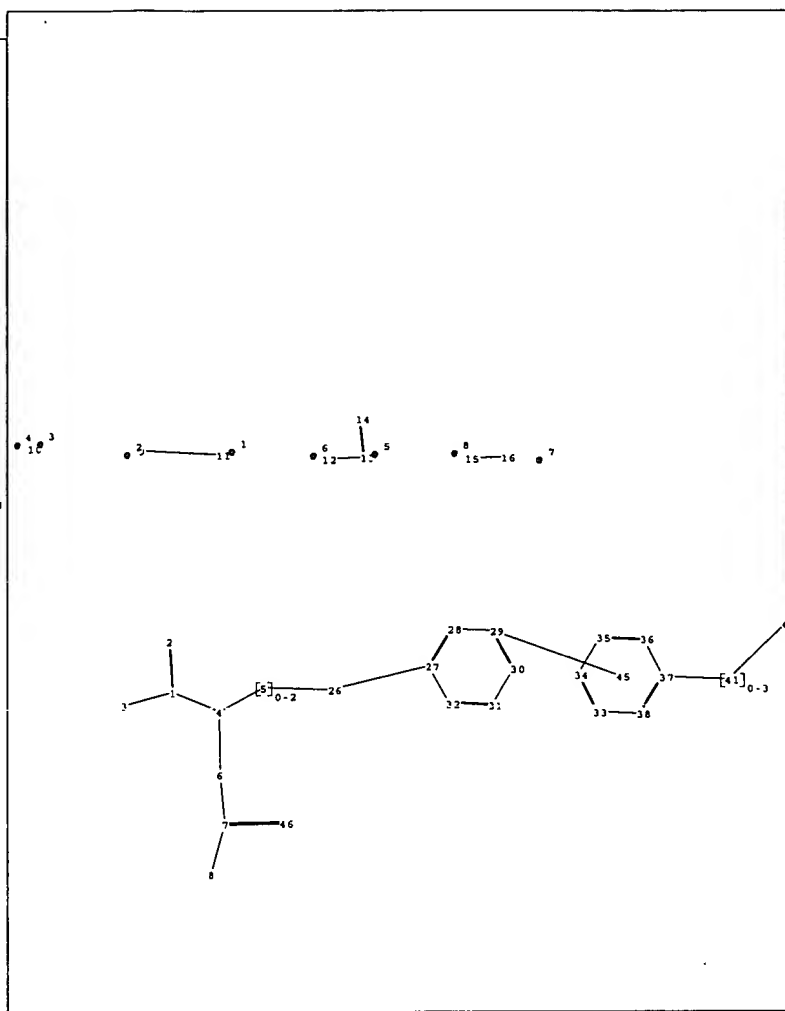
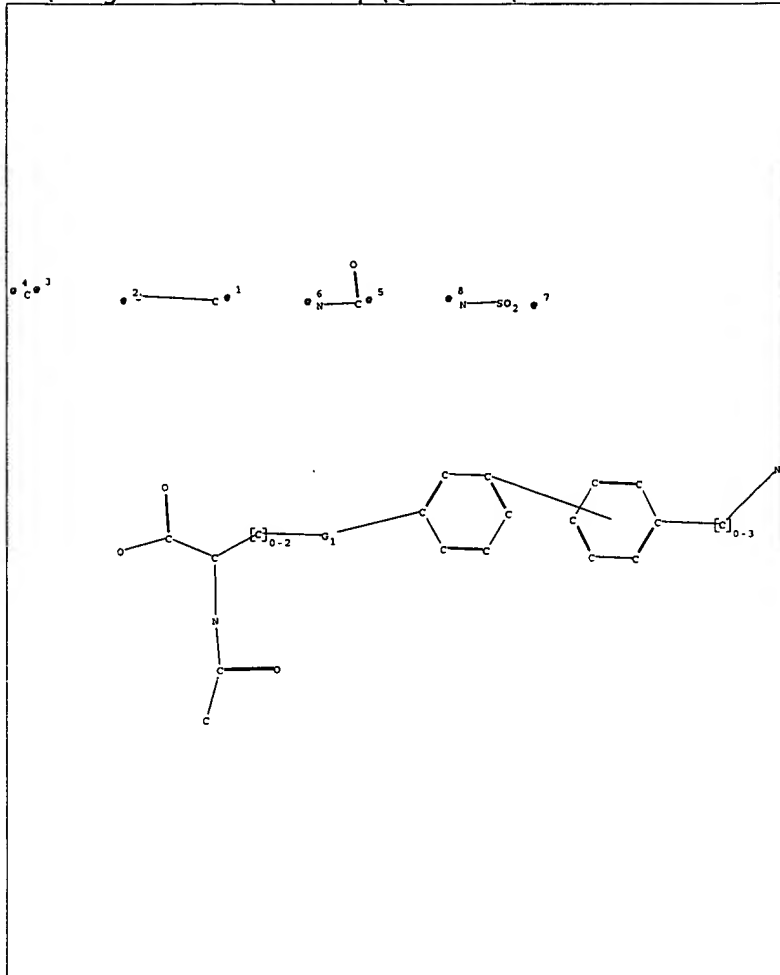
normalized bonds :

27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38

G1: [\*1-\*2], [\*3-\*4], [\*5-\*6], [\*7-\*8]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 26:CLASS 27:Atom 28:Atom  
 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom  
 41:CLASS 42:CLASS 43:CLASS



chain nodes :

1 2 3 4 5 6 7 9 10 11 12 13 14 15 16 26 41 46

ring nodes :

27 28 29 30 31 32 33 34 35 36 37 38

ring/chain nodes :

8 42

chain bonds :

1-2 1-3 1-4 4-5 4-6 5-26 6-7 7-8 7-46 9-11 12-13 13-14 15-16 26-27 37-41  
41-42

ring bonds :

27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38

exact/norm bonds :

1-2 1-3 4-6 5-26 6-7 7-46 12-13 13-14 15-16 26-27 41-42

exact bonds :

1-4 4-5 7-8 9-11 37-41

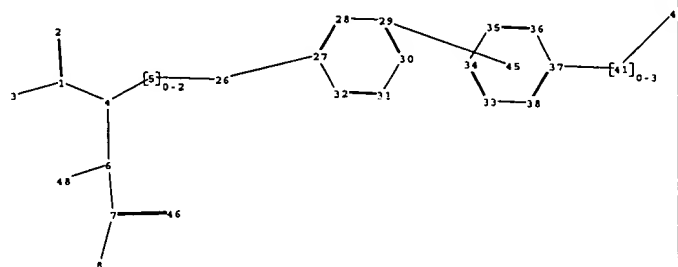
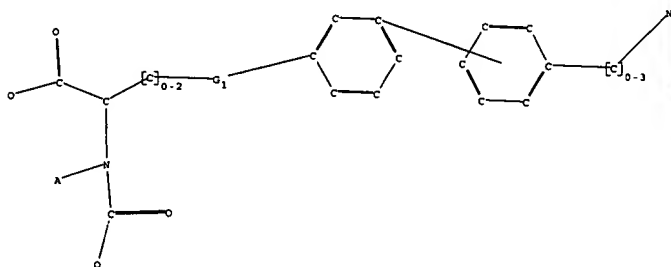
normalized bonds :

27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38

G1: [\*1-\*2], [\*3-\*4], [\*5-\*6], [\*7-\*8]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 26:CLASS 27:Atom 28:Atom  
29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom  
41:CLASS 42:CLASS 45:CLASS 46:CLASS



chain nodes :

1 2 3 4 5 6 7 9 10 11 12 13 14 15 16 26 41 46 48

ring nodes :

27 28 29 30 31 32 33 34 35 36 37 38

ring/chain nodes :

8 42

chain bonds :

1-2 1-3 1-4 4-5 4-6 5-26 6-7 6-48 7-8 7-46 9-11 12-13 13-14 15-16 26-27  
37-41 41-42

ring bonds :

27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38

exact/norm bonds :

1-2 1-3 4-6 5-26 6-7 6-48 7-8 7-46 12-13 13-14 15-16 26-27 41-42

exact bonds :

1-4 4-5 9-11 37-41

normalized bonds :

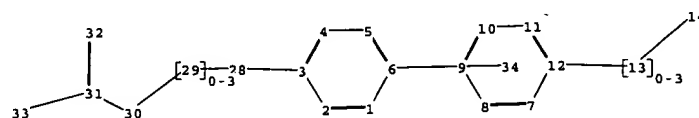
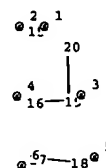
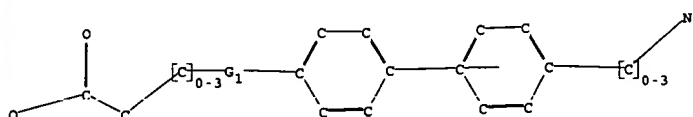
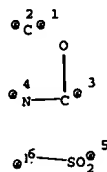
27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38

G1:[\*1-\*2],[\*3-\*4],[\*5-\*6],[\*7-\*8]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 26:CLASS 27:Atom 28:Atom  
29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom  
41:CLASS 42:CLASS 45:CLASS 46:CLASS 48:CLASS





chain nodes :

13 15 16 17 18 19 20 28 29 30 31 32 33

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

14

chain bonds :

3-28 12-13 13-14 16-19 17-18 19-20 28-29 29-30 30-31 31-32 31-33

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

3-28 13-14 16-19 17-18 19-20 28-29 31-32 31-33

exact bonds :

12-13 29-30 30-31

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1: [\*1-\*2], [\*3-\*4], [\*5-\*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS  
 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS